

On Arrangements of Six, Seven, and Eight Spheres: Maximal Bonding of Monatomic Ionic Compounds

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Abstract

Let $C(n)$ be the solution to the contact number problem: the maximum number of touching pairs among any packing of n congruent spheres in \mathbb{R}^3 . We prove the long conjectured values of $C(6) = 12$, $C(7) = 15$, and $C(8) = 18$. The proof strategy generalizes under an extensive case analysis to $C(9) = 21$, $C(10) = 25$, $C(11) = 29$, $C(12) = 33$, and $C(13) = 36$. These results have great import for condensed matter physics, materials science, physical chemistry of interfaces, and organic crystal engineering.

The Chemical Interpretation of Contact Numbers

The contact number problem has been extensively studied by mathematicians, condensed matter physicists, and materials scientists [1], [2], [3] [4], [5], [6], [7], [8], [9], [10], with important applications in physics, chemistry, and biology, [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21]. This work has discovered proofs of the putative values of $C(n)$ for $n < 14$. In this paper we present explicit written proofs for $C(6) = 12$, $C(7) = 15$, and $C(8) = 18$. The proofs for $8 < n < 14$ leading to the values of $C(9) = 21$, $C(10) = 25$, $C(11) = 29$, $C(12) = 33$, $C(13) = 36$ are very lengthy and will be transcribed from a *Mathematica* notebook into explicit written proofs shortly; however the most elegant and insightful instantiations of the proof technique are found for $5 < n < 9$, and the writing ends here in order to not obfuscate the main idea with hundreds of pages of case analysis.

Theorem 1. *Let A_Z be an ionic monatomic A compound with Z atoms. Then A_Z has at most $C(Z)$ chemical bonds. In particular, A_6 has at 12 chemical bonds, A_7 has at most 15 chemical bonds, A_8 has at most 18 chemical bonds, A_9 has at most 21 chemical bonds, A_{10} has at most 25 chemical bonds, A_{11} has at most 29 chemical bonds, A_{12} has at most 33 chemical bonds, and A_{13} has at most 36 chemical bonds.*

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This is true for any atom A , and more generally, for Z non-overlapping congruent moieties; this generalization to moieties is of great importance for organic chemistry. For functional groups can be considered as a moiety that is approximable to a sphere, implying that steric hindrance and the theoretical calculation of Ramachandran plots can be achieved using contact numbers as opposed to x-ray crystallography; applied discrete geometry at work [3].

Six Spheres

Theorem 2.

$$C(6) = 12.$$

Proof. Assume to the contrary that $C(6) \geq 13$. Then there exists a sphere packing

$$\mathcal{P} = \bigcup_{i=1}^6 (x_i + \mathbb{S}^2) \hookrightarrow \mathbb{R}^3$$

with $V(\mathcal{P}) = \{x_1, x_2, x_3, x_4, x_5, x_6\}$ and $|E(\mathcal{P})| \geq 13$. By the Handshaking Lemma,

$$\frac{1}{2} \sum_{i=1}^6 \deg x_i \geq 13, \text{ and hence, } \sum_{i=1}^6 \deg x_i \geq 26.$$

Assume that

$$\max_{1 \leq i \leq 6} \deg x_i \leq 4.$$

Hence, we obtain the following contradiction:

$$\sum_{i=1}^6 \deg x_i \leq 6 \cdot 4 = 24 < 26.$$

Thus,

$$5 \leq \max_{1 \leq i \leq 6} \deg x_i < 6,$$

since $|V(\mathcal{P})| = 6$, and $\exists 1 \leq j \leq 6, \deg x_j = 5$. Assume that

$$\max_{i \neq j} \deg x_i \leq 4.$$

Hence, we obtain the following contradiction:

$$\sum_{i \neq j} \deg x_i \leq 5 \cdot 4 = 20 < 21.$$

Thus,

$$5 \leq \max_{i \neq j} \deg x_i < 6,$$

so there are at least two spheres of exactly degree 5. Without loss of generality, say that $\deg x_5 = \deg x_6 = 5$. Hence,

$$\sum_{i=1}^4 \deg x_i \geq 26 - 2 \cdot 5 = 16.$$

No other spheres have degree 5, so at most 2 spheres have degree 4, and the other two spheres have at most degree 3, so $2 \cdot 4 + 2 \cdot 3 = 14 < 16$, which is a contradiction. Therefore, $C(6) = 12$. \square

Seven Spheres

Theorem 3.

$$C(7) = 15.$$

Proof. Assume to the contrary that $C(7) \geq 16$. Then there exists a sphere packing

$$\mathcal{P} = \bigcup_{i=1}^7 (x_i + \mathbb{S}^2) \hookrightarrow \mathbb{R}^3$$

with $V(\mathcal{P}) = \{x_1, x_2, x_3, x_4, x_5, x_6, x_7\}$ and $|E(\mathcal{P})| \geq 16$. By the Handshaking Lemma,

$$\frac{1}{2} \sum_{i=1}^6 \deg x_i \geq 16, \text{ and hence, } \sum_{i=1}^6 \deg x_i \geq 32.$$

Now,

$$5 \leq \max_{1 \leq i \leq 7} \deg x_i \leq 6.$$

Lemma 1. *There are at most two spheres of degree 6 in \mathcal{P} , and if there are two spheres of degree 6 in \mathcal{P} , then there can be no sphere of degree 5 in \mathcal{P} .*

Lemma 2. *If a sphere of degree 6 in \mathcal{P} touches two spheres of degree 5 in \mathcal{P} , then there is a sphere of degree 3 in \mathcal{P} .*

Lemma 3. *If there are two spheres of degree 6 in \mathcal{P} , then there are at most three spheres of degree 4 in \mathcal{P} .*

Lemma 4. *If a sphere of degree 6 in \mathcal{P} touches a sphere of degree 5 in \mathcal{P} , then there is at most one other sphere of degree 5 in \mathcal{P} .*

Lemma 5. *Any two spheres of degree 5 in \mathcal{P} which do not touch, simultaneously touch three spheres of degree 5 in \mathcal{P} , and every sphere of degree 5 in \mathcal{P} touches four other spheres of degree 5 in \mathcal{P} .*

Lemma 6. *Any two spheres of degree 4 in \mathcal{P} cannot simultaneously touch any two touching spheres of degree 5 in \mathcal{P} .*

Case 1. $\max_{1 \leq i \leq 7} \deg x_i = 6$.

Subproof. Then, $\sum_{i=1}^6 \deg x_i \geq 26$. Furthermore, without loss of generality,

(a) $\max_{1 \leq i \leq 6} \deg x_i = 6$.

Subproof. Then, $\sum_{i=1}^5 \deg x_i \geq 20$. Furthermore, without loss of generality,

- i. $\max_{1 \leq i \leq 5} \deg x_i = 6$. Then, $\sum_{i=1}^4 \deg x_i \geq 14$. Hence, the degree sequence is either $(6, 6, 6, 5, 3, 3, 3)$ or $(6, 6, 6, 4, 4, 3, 3)$, which contradicts Lemmas 1-4.
- ii. $\max_{1 \leq i \leq 5} \deg x_i = 5$. Then, $\sum_{i=1}^4 \deg x_i \geq 15$. Hence, the degree sequence is either $(6, 6, 5, 5, 4, 3, 3)$ or $(6, 6, 5, 4, 4, 4, 3)$, which contradicts Lemmas 1-4.
- iii. $\max_{1 \leq i \leq 5} \deg x_i = 4$. Hence, the degree sequence is $(6, 6, 4, 4, 4, 4, 4)$, which contradicts Lemmas 1-4.

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(b) $\max_{1 \leq i \leq 6} \deg x_i = 5$.

Subproof. Then, $\sum_{i=1}^5 \deg x_i \geq 21$. Furthermore, without loss of generality,

$$\max_{1 \leq i \leq 5} \deg x_i = 5 \Rightarrow \sum_{i=1}^4 \deg x_i \geq 16$$

i. $\max_{1 \leq i \leq 4} \deg x_i = 5$.

Subproof. Then, $\sum_{i=1}^3 \deg x_i \geq 11$. Hence, the degree sequence is either $(6, 5, 5, 5, 5, 3, 3)$ or $(6, 5, 5, 5, 4, 4, 3)$, which contradicts Lemmas 1-4.

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ii. $\max_{1 \leq i \leq 4} \deg x_i = 4$.

Subproof. Then, $\sum_{i=1}^3 \deg x_i \geq 12$. Hence, the degree sequence is $(6, 5, 5, 4, 4, 4, 4)$, which contradicts Lemmas 1-4.

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Case 2. $\max_{1 \leq i \leq 7} \deg x_i = 5$.

Subproof. Then, $\sum_{i=1}^6 \deg x_i \geq 27$. Furthermore, without loss of generality,

$$\max_{1 \leq i \leq 6} \deg x_i = 5 \Rightarrow \sum_{i=1}^5 \deg x_i \geq 22$$

$$\max_{1 \leq i \leq 5} \deg x_i = 5 \Rightarrow \sum_{i=1}^4 \deg x_i \geq 17$$

$$\max_{1 \leq i \leq 4} \deg x_i = 5 \Rightarrow \sum_{i=1}^3 \deg x_i \geq 12$$

(a) $\max_{1 \leq i \leq 3} \deg x_i = 5$.

Subproof. Then, $\deg x_1 + \deg x_2 \geq 7$. Hence, the degree sequence is either $(5, 5, 5, 5, 5, 5, 2)$ or $(5, 5, 5, 5, 5, 4, 3)$, which contradicts Lemma 5. ◁

(b) $\max_{1 \leq i \leq 3} \deg x_i = 4$.

Subproof. Then $\deg x_1 + \deg x_2 \geq 8$, so $\deg x_1 = \deg x_2 = 4$. Hence, the degree sequence is $(5, 5, 5, 5, 4, 4, 4)$, which contradicts Lemma 6. ◁

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Eight Spheres

Theorem 4.

$$C(8) = 18.$$

Proof. Assume to that contrary that $C(8) \geq 19$. Then there exists a sphere packing

$$\mathcal{P} = \bigcup_{i=1}^8 (x_i + \mathbb{S}^2) \hookrightarrow \mathbb{R}^3$$

with $V(\mathcal{P}) = \{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8\}$ and $|E(\mathcal{P})| \geq 19$. By the Handshaking Lemma,

$$\frac{1}{2} \sum_{i=1}^8 \deg x_i \geq 19, \text{ and hence, } \sum_{i=1}^8 \deg x_i \geq 38.$$

Now,

$$5 \leq \max_{1 \leq i \leq 8} \deg x_i \leq 7.$$

Case 1. $\max_{1 \leq i \leq 8} \deg x_i = 7$.

Subproof. Then $\sum_{i=1}^7 \deg x_i \geq 31$. Furthermore, without loss of generality,

(a) $\max_{1 \leq i \leq 7} \deg x_i = 7$.

Subproof. Then $\sum_{i=1}^6 \deg x_i \geq 24$. Furthermore, without loss of generality,

i. $\max_{1 \leq i \leq 6} \deg x_i = 7$.

Subproof. Then $\sum_{i=1}^5 \deg x_i \geq 17$. Hence, the degree sequence is either $(7, 7, 7, 5, 3, 3, 3, 3)$ or $(7, 7, 7, 4, 4, 3, 3, 3)$, which is a contradiction. \triangleleft

ii. $\max_{1 \leq i \leq 6} \deg x_i = 6$.

Subproof. Then $\sum_{i=1}^5 \deg x_i \geq 18$. Hence, the degree sequence is either $(7, 7, 6, 6, 3, 3, 3, 3)$, $(7, 7, 6, 5, 4, 3, 3, 3)$, or $(7, 7, 6, 4, 4, 4, 3, 3)$, which is a contradiction. \triangleleft

iii. $\max_{1 \leq i \leq 6} \deg x_i = 5$.

Subproof. Then $\sum_{i=1}^5 \deg x_i \geq 19$. Hence, the degree sequence is either $(7, 7, 5, 5, 5, 3, 3, 3)$, $(7, 7, 5, 5, 4, 4, 3, 3)$, or $(7, 7, 5, 4, 4, 4, 4, 3)$, which is a contradiction. \triangleleft

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(b) $\max_{1 \leq i \leq 7} \deg x_i = 6$.

Subproof. Then $\sum_{i=1}^6 \deg x_i \geq 25$. Furthermore, without loss of generality,

i. $\max_{1 \leq i \leq 6} \deg x_i = 6$.

Subproof. Then $\sum_{i=1}^5 \deg x_i \geq 19$. Hence, the degree sequence is either $(7, 6, 6, 6, 4, 3, 3, 3)$, $(7, 6, 6, 5, 5, 3, 3, 3)$, or $(7, 6, 6, 4, 4, 4, 4, 3)$, which is a contradiction. \triangleleft

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ii. $\max_{1 \leq i \leq 6} \deg x_i = 5$.

Subproof. Then $\sum_{i=1}^5 \deg x_i \geq 20$. Hence, the degree sequence is $(7, 6, 5, 4, 4, 4, 4, 4)$, which is a contradiction. \triangleleft

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(c) $\max_{1 \leq i \leq 7} \deg x_i = 5$.

Subproof. Then $\sum_{i=1}^6 \deg x_i \geq 26$. Hence, the degree sequence is either $(7, 5, 5, 5, 5, 5, 3, 3)$, $(7, 5, 5, 5, 5, 4, 4, 3)$, or $(7, 5, 5, 5, 4, 4, 4, 4)$, which is a contradiction. \triangleleft

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Case 2. $\max_{1 \leq i \leq 8} \deg x_i = 6$.

Subproof. Then $\sum_{i=1}^7 \deg x_i \geq 32$. Furthermore, without loss of generality,

(a) $\max_{1 \leq i \leq 7} \deg x_i = 6$.

Subproof. Then $\sum_{i=1}^6 \deg x_i \geq 26$. Hence, the degree sequence is either $(6, 6, 6, 6, 5, 3, 3, 3)$, $(6, 6, 6, 6, 4, 4, 3, 3)$, $(6, 6, 6, 5, 5, 4, 3, 3)$, $(6, 6, 6, 5, 4, 4, 4, 3)$, $(6, 6, 6, 4, 4, 4, 4, 4)$, or $(6, 6, 5, 5, 4, 4, 4, 4)$, which is a contradiction. \triangleleft

(b) $\max_{1 \leq i \leq 7} \deg x_i = 5$.

Subproof. Then $\sum_{i=1}^6 \deg x_i \geq 27$. Hence, the degree sequence is either $(6, 5, 5, 5, 5, 4, 4, 4)$ or $(6, 5, 5, 5, 5, 5, 4, 3)$, which is a contradiction. \triangleleft

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Case 3. $\max_{1 \leq i \leq 8} \deg x_i = 5$.

Subproof. Then $\sum_{i=1}^7 \deg x_i \geq 33$. Hence, the degree sequence is either $(5, 5, 5, 5, 5, 5, 5, 3)$ or $(5, 5, 5, 5, 5, 5, 4, 4)$, which is a contradiction. \triangleleft

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